Tetradecane

629-59-	4 DTXSID1	02726

Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 252 °C

Global applicability domain: Inside

Local applicability domain index: 6.94e-01

Confidence level: 8.39e-01

Nearest Neighbors from the Training Set

Image not found

Tetradecane Measured: 254 Predicted: 252 Image not found

1-Tetradecene Measured: 233 Predicted: 243 Image not found

Pentadecane Measured: 271 Predicted: 269

Image not found

Tridecane Measured: 235 Predicted: 231 Image not found

Cyclohexane, octyl-Measured: 264 Predicted: 263